

Description of Additional Supplementary Files

Supplementary Movie. 1 | SMD simulated trajectories for pulling the 2C TCR–SIYR:H2-K^b complex. The C-terminal residue of H-2K^b was harmonically constrained and the C terminus of TCR was pulled by a dummy spring moving at ~0.1 nm/ns with a spring constant of ~70 pN/nm. The color codes were the same as that in Figure 7a,b and 2C TCR α (blue), 2C TCR β (red), MHC H-2K^b α (orange), MHC H-2K^b β 2m (cyan), and R4 peptide (green). Three different pathways of conformational changes were observed in the pMHC.

Supplementary Movie. 2 | CMD and SMD simulated trajectories side-by-side comparison of pulling effect on the human TCR-CD3 complex focusing on interaction of P223 (TCR β) and L90 (CD3 ϵ). The left panel shows the freely evolved fluctuations without force from CMD, and the right panel presents the constrained dynamics with force from SMD. For SMD trajectory, the external force of 175pN was exerted on the N-terminal of TCR α , pulling upwards while keeping the C-termini of CD3 ϵ anchored. The color codes were the same as that in Fig. 7g: TCR α (yellow-green), TCR β (green), and CD3 subunits (golden). The focused interacting residues were highlighted using spheres, where P223 β (red) was pulled closer to L90 ϵ (gray) in the presence of force.

Supplementary Movie. 3 | CMD and SMD simulated trajectories side-by-side comparison of pulling effect on the human TCR-CD3 complex focusing on interaction of K183 (TCR β) and L90 (CD3 ϵ ’). The left panel shows the freely evolved fluctuations without force from CMD, and the right panel presents the constrained dynamics with force from SMD. For SMD trajectory, the external force of 175pN was exerted on the N-terminal of TCR α , pulling upwards while keeping the C-termini of CD3 ϵ anchored. The color codes were the same as that in Fig. 7g: TCR α (yellow-green), TCR β (green), and CD3 subunits (golden). The focused interacting residues were highlighted using spheres, where K183 β (blue) was pulled away from L90 ϵ ’ (gray) in the presence of force.

Supplementary Movie. 4 | CMD and SMD simulated trajectories side-by-side comparison of pulling effect on the human TCR-CD3 complex focusing on interaction of N225 (TCR β) and E38 (CD3 γ). The left panel shows the freely evolved fluctuations without force from CMD, and the right panel presents the constrained dynamics with force from SMD. For SMD trajectory, the external force of 175pN was exerted on the N-terminal of TCR α , pulling upwards while keeping the C-termini of CD3 ϵ anchored. The color codes were the same as that in Fig. 7g: TCR α (yellow-green), TCR β (green), and CD3 subunits (golden). The focused interacting residues were highlighted using spheres, where N225 β (purple) was pulled away from E38 γ (gray) in the presence of force.